

SCD Manual

Linux Version

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[Note: Filenames and directories are *italic*. Commands and programs are **bold**.]

Data analysis

Currently one needs to load a run file with ISAW, and then run **peaks** from the appropriate menu, which creates a separate peaks file for each histogram. This still needs to be worked on, but ideally this will create a single *expnam.x* file and a *expnam.peaks* file for each experiment.

At this time, programs which have been ported from the VAX to the Linux computer include:

```
blind
scalar
index
lsqrs
```

This allows one to determine the unit cell and orientation matrix, and get started with data collection. The programs work pretty much the same way as on the VAX. Other programs which have been ported to Linux are **htox**, **setang**, **wlcalc** and **xtoh**.

The binaries (executables) are stored in */IPNShome/scd/bin*. To run one of these programs, you first need to log on to the Linux cluster under your username, and set the path to include the directory containing the binaries:

```
[...]$ export PATH=$PATH:/IPNShome/scd/bin
```

So you do not have to type in this command each time you log on, use a text editor to add the export command to the end of your *.bashrc* file.

Alternatively, you can create a */bin* directory in you own account and then copy the executables to your own account:

```
[user@helios user]$ mkdir bin
[user@helios user]$ cd bin
[user@helios bin]$ cp /IPNShome/scd/bin/* ./
```

Other scd subdirectories that you may want to read or copy if you are doing program development are */src*, */subs*, */lib*, and */INCLDS*.

If you want to do a test drive of the software beginning with **blind**, copy the contents of the */IPNShome/scd/quartz* directory to your account. The *quartz.peaks* file is a text file (*v.i.*) which you can view with the **more** command or with a text editor.

Compiling and linking Fortran source code

```
g77 program.f -o program /IPNShome/scd/lib/scdlib.a
```

This command links to the subroutine object library *scdlib.a*, which is stored in the */IPNShome/lib* directory.

If your current directory is */IPNShome/scd/scdsubs*, then all the subroutines can be compiled and linked by typing **makelib**, which is a script file stored in */IPNShome/bin*. The commands in **makelib** are:

```
#!/bin/sh
g77 -c *.f -w
ar -r /IPNShome/lib/scdlib.a *.o
rm *.o
```

This compiles all the *.f files, writes the object files into *scdlib.a* (replaces old object files with the new ones), and deletes the object files in the */IPNShome/scdsubs* directory.

To list the entries in the library, type

```
ar -t /IPNShome/lib/scdlib.a
```

Experiment files

These are “keyed” files which simulate the key-access ISAM files on DEC VMS computers. Most of the I/O routines are borrowed from GSAS code.

For now, SCD experiment files, previously *expnam.exp* files on the SCD computer, are named *expnam.x* files to keep them separate from GSAS *expnam.exp* files. At some point we plan to merge keys so that the same *exp* file is compatible with SCD software and with GSAS.

If you edit the *expnam.x* file using a text editor, then you must run **cnvfile**.

```
[... ]$ cnvfile  
Enter datafile to convert to GSAS format >expnam.x  
Enter datafile to convert to GSAS format >␣
```

Peaks files

Output from **peaks** is *expnam.peaks*. This is a text (ASCII) file. The first character of each record (0, 1, 2 or 3) defines the type of data and the format for the record. The following is a portion of a peaks file showing how data from consecutive runs are appended to the file.

```

0  NRUN DETNUM   DETA   DETA2   DETD   CHI   PHI   OMEGA   MONCNT
1  6496      1  90.00    0.00   32.00  167.00   0.00   45.00  138568
2  SEQN   H   K   L       X       Y       Z   XCM   YCM   WL   IPK   INTI   SIGI  RFLG   NRUN  DN
3    1    2    7    2   9.01  27.95  13.12 -10.02  -4.37  0.6085  23   0.00   0.00    1  6496  1
3    2    3    6    2   8.95  43.76  15.28 -10.03   0.55  0.6285  25   0.00   0.00    1  6496  1
3    3    4    6    1  31.93  54.15  18.22  -3.28   3.78  0.6575  28   0.00   0.00    1  6496  1
3   20    2    4    0  52.90  43.11  58.40   2.89   0.34  1.1934  66   0.00   0.00    1  6496  1
3   21    1    3    1   4.87  32.83  66.12 -11.23  -2.85  1.3355  30   0.00   0.00    1  6496  1
3   22    2    3    0  52.81  55.84  71.26   2.86   4.30  1.4441 154   0.00   0.00    1  6496  1
3   23    1    3    0  52.84  29.95  84.11   2.87  -3.75  1.7478 356   0.00   0.00    1  6496  1
3   24    2    2    0  48.78  74.77  85.94   1.68  10.19  1.7939 272   0.00   0.00    1  6496  1
3   25    1    2    0  52.93  43.10 105.09   2.90   0.34  2.3882 160   0.00   0.00    1  6496  1
0  NRUN DETNUM   DETA   DETA2   DETD   CHI   PHI   OMEGA   MONCNT
1  6497      1  90.00    0.00   32.00  167.00  90.00   45.00  152156
2  SEQN   H   K   L       X       Y       Z   XCM   YCM   WL   IPK   INTI   SIGI  RFLG   NRUN  DN
3   26   -2    0   12   9.94  58.81   4.10  -9.74   5.23  0.5325  21   0.00   0.00    0  6497  1
3   27   -3    2   10  26.92  29.97  19.95  -4.75  -3.74  0.6744  24   0.00   0.00    1  6497  1

```

Reflection are read by a call to subroutine *readrefl*. If the records are being modified, such as changing the hkl's in **index**, then the call is to *readref2*.

Glossary:

NRUN	run number
DETNUM	detector number
DETA	detector angle in the horizontal plane
DETA2	detector angle out of the horizontal plane
CHI	chi angle
PHI	phi angle
OMEGA	omega angle, fixes at 45 deg.
MONCNT	incident beam detector monitor counts
SEQN	sequence number
H,K,L	h,k,l
X,Y,Z	histogram channels
XCM,YCM	distance from the detector center in centimeters
WL	wavelength in Angstroms
IPK	neutron counts at peak maximum
INTI	integrated peak intensity
SIGI	sigma for INTI based on counting statistics
RFLG	reflection flag, usually equal to the crystal number
NRUN	run number again
DN	detector number again, same as DETNUM

Data analysis on Windows pc computers

All of the above programs can be compiled using **g77** in a MS-DOS command window on a Windows pc computer. In fact, this might be the way to go in the future – as with GSAS, users will install all programs on their own pc to which they download the data for analysis.

On my pc, I created the following folders which mirror those on the SCD Linux computer:

```
c:\scd
c:\scd\bin
c:\scd\INCLDS
c:\scd\lib
c:\scd\quartz
c:\scd\scdsrc
c:\scd\scdsubs
```

In the *scdsubs* subdirectory, I created a *makelib.bat* file with the following commands:

```
g77 -c *.f
ar -r scdlib.a *.o
move scdlib.a c:\scd\lib\
@echo off
echo.
```

This will compile all of the subroutines and make a library.

In the *scdsrc* subdirectory, for each program type

```
g77 program.f -o program c:\scd\lib\scdlib.a
```

Then move the *program.exe* files to the *bin* subdirectory. One could also make a *bat* file to do all of this at once.

Of course, to compile programs on your pc you will need to obtain the **g77** compiler. See the SCD web page (<http://www.pns.anl.gov/SCD/scd2.html>) and then click on “GNU Fortran G77 for Win32.”

For general users who just want the program executables, I will establish an ftp site for users to download executables. Then they could download the programs to a folder, such as *c:\scd\bin*, which should be included in their PATH statement.